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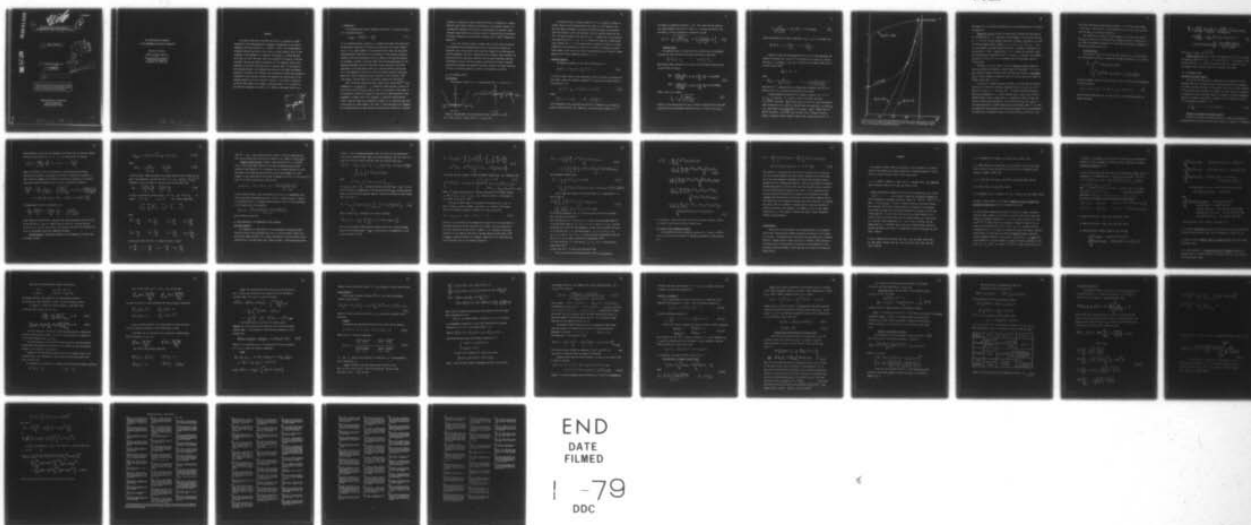
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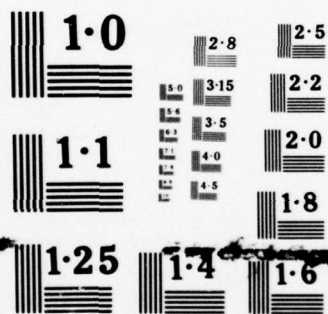
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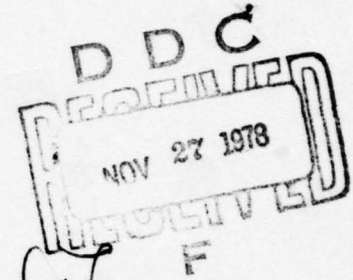
**THE SEMICLASSICAL EXPANSION OF
THE ANHARMONIC-OSCILLATOR PROPAGATOR.**

10 Maurice M. Mizrahi

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JOB

THE SEMICLASSICAL EXPANSION
OF THE ANHARMONIC-OSCILLATOR PROPAGATOR¹

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ABSTRACT

This paper shows how to calculate the terms of a semiclassical (WKB) expansion of the quantum-mechanical propagator corresponding to the quartic anharmonic-oscillator potential, $V = m\omega^2 q^2/2 + \lambda q^4/4$. This nonperturbative treatment expresses each term in the series as a path integral, which is then evaluated in the framework of a formalism, introduced by C. DeWitt-Morette, which does not entail the usual time-slicing operation followed by a limiting procedure. The Gaussian measure used absorbs all the quadratic terms in the expansion of the action functional about a classical path. The covariance of this Gaussian measure is the Feynman Green function of the small-disturbance operator of the system. This function can be obtained by varying the constants of integration in the classical solution, and therefore the coefficients of the expansion depend only on this classical solution. If the latter is chosen to be the one which tends to its harmonic counterpart when $\lambda \rightarrow 0$, then it is seen that the propagator also tends to its harmonic counterpart when $\lambda \rightarrow 0$.

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I. INTRODUCTION

The one-dimensional quartic anharmonic oscillator is a particle of mass m in a potential given by:

$$V(q) = \frac{m\omega^2 q^2}{2} + \frac{\lambda q^4}{4}. \quad (1)$$

It is an important model in physics as a prototype nonlinear field theory and has generated a great deal of activity in recent years for several reasons. First, it is a simple example of a perturbation which causes the associated quantum-mechanical quantities to be non-analytic in the coupling constant λ . Therefore, the usual perturbation series in powers of the coupling constant are divergent, although it has been shown² that the Padé approximants of the Rayleigh-Schrödinger series for the energy levels converge to the correct eigenvalues of the Hamiltonian, which has a positive-definite spectrum for $\lambda > 0$. The anharmonic oscillator is also the simplest nonlinear interaction which still yields plane-wave periodic solutions in the associated $\lambda\phi^4$ field theory, and even admits of a restricted superposition principle³.

While the energy spectrum has been studied rather extensively^{2,4,5}, the propagator $K \equiv \langle q_b, t_b | q_a, t_a \rangle$, or probability amplitude that a particle at q_a at time t_a will be at q_b at time t_b , has not. The purpose of this paper is to show how to calculate the terms of a semiclassical (WKB) expansion of this propagator (in powers of \hbar). This treatment, of necessity nonperturbative since it does not hinge on any expansion in powers of λ , expresses each term in the series as a path integral. The latter is then evaluated in the framework of a formalism where the usual approach of time-slicing followed by a limiting

procedure is replaced by a more tractable definition, introduced by C. DeWitt-Morette⁶, which greatly simplifies calculations. This approach enabled us to systematically generate all the terms in the semiclassical expansion, which represents some progress over previous studies of approximating the anharmonic oscillator propagator by path-integral techniques (Lam⁷, Sarkar⁸, Mathews and Seshadri⁹).

First, the classical system is studied: the classical paths joining two fixed endpoints are calculated and the limit of zero coupling constant is discussed. Then, the classical action and other elements of the WKB expansion (Jacobi commutator, Van Vleck - Morette function, Feynman's Green function) are derived explicitly, and their connection with the small-disturbance equation investigated. Finally, the path integrals constituting the terms of the WKB expansion are exhibited and reduced to definite integrals over known functions, first for an arbitrary potential, then for the anharmonic oscillator.

II. THE CLASSICAL SYSTEM

The Potential

The potential, given in (1), is sketched below for $\lambda > 0$ and $\lambda < 0$.

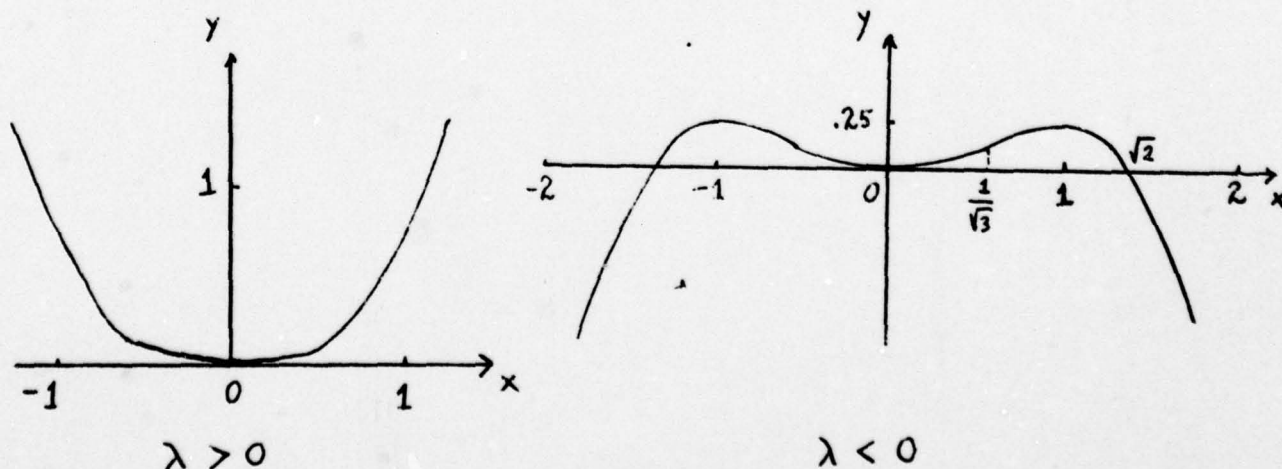


Figure 1. The anharmonic oscillator potential $V(q) = m\omega^2 q^2/2 + \lambda q^4/4$
 $[y = x^2/2 \pm x^4/4; y \equiv V(q)|\lambda|/m^2\omega^4, x \equiv q|\lambda|^{1/2}/\omega m^{1/2}]$.

The potential well is always present for $\lambda < 0$, so there will always be harmonic motion in some neighborhood of the origin. As $|\lambda|$ decreases, the well gets deeper and deeper, the maxima go higher and higher, and the points where the potential crosses the horizontal axis are rejected farther and farther. The drastic change in the shape of V as λ changes sign is the cause for the nonanalyticity in λ . For $\lambda > 0$, there will always be a stable ground state, whereas for $\lambda < 0$, the ground state is unstable, as there is a finite probability for the particle to "leak out" of the well. The failure of perturbation theory is due to the fact that at large distances the q^4 term will always dominate the q^2 term, regardless how small λ is.

Dynamical Equation

The dynamical equation for the classical path $q_c(t)$ is:

$$\ddot{q}_c(t) + \omega^2 q_c(t) + \frac{\lambda}{m} q_c^3(t) = 0. \quad (2)$$

It can be solved in terms of the (biperiodic) elliptic functions. Our source for the latter is Byrd and Friedman's handbook¹⁰. We choose the following form for the solution of (2):

$$q_c(t) = q_m \operatorname{cn}[\Omega(t - t_0), k], \quad (3)$$

where

$$\Omega^2 \equiv \omega^2 + \lambda q_m^2, \quad k^2 \equiv \frac{\lambda}{2} \left(\frac{q_m}{\omega} \right)^2.$$

This corresponds to the case where the particle is released at q_m at time $t=t_0$ with no initial velocity. (For simplicity, we take the mass m equal to 1; it

can always be restored by replacing λ by λ/m). Note that the modulus k lies always between 0 and $1/\sqrt{2}$ ($= 0.707\dots$). If we take the modulus k and the phase t_0 to be our constants of integration, we get:

$$q_c(t) = \sqrt{\frac{2k^2\omega^2}{\lambda(1-2k^2)}} \operatorname{cn} \left[\frac{\omega(t-t_0)}{\sqrt{1-2k^2}}, k \right]. \quad (4)$$

Classical paths

The classical paths of interest for the calculation of the propagator are those for which the initial and final positions are specified:

$$q_c(t_a) = q_a \quad ; \quad q_c(t_b) = q_b.$$

Substituting these conditions in (4) yields the relationship between the set (k, t_0) and the set (q_a, q_b) :

$$\begin{aligned} (a) \quad \frac{\omega(t_a - t_0)}{\sqrt{1-2k^2}} &= \pm \operatorname{cn}^{-1} \left(\frac{q_a}{q_m}, k \right) + 4nK(k) \\ (b) \quad \frac{\omega(t_b - t_0)}{\sqrt{1-2k^2}} &= \pm \operatorname{cn}^{-1} \left(\frac{q_b}{q_m}, k \right) + 4n'K(k), \end{aligned} \quad (5)$$

where n and n' are integers,

$$q_m \equiv \sqrt{\frac{2k^2\omega^2}{\lambda(1-2k^2)}}, \quad (6)$$

and $K(k)$ is the quarter-period of the cn function. Subtracting (5a) from (5b) yields the final transcendental equations giving k in terms of q_a and q_b :

$$\pm \frac{\omega T}{\sqrt{1-2k^2}} = \varphi_{\pm}(k^2) + 4NK(k), \quad (7)$$

where any combination of signs is permitted, $T \equiv t_b - t_a$, N is an integer, and

$$\varphi_{\pm}(k^2) \equiv \operatorname{cn}^{-1}\left(\frac{q_a}{q_m}\right) \pm \operatorname{cn}^{-1}\left(\frac{q_b}{q_m}\right).$$

Equation (7) must be solved graphically for k (t_0 is then determined, for example, by Equation 5a). Since $\operatorname{cn}^{-1}u$ is defined only for $u \in [-1, 1]$, we must have $|q_a| \leq q_m$ and $|q_b| \leq q_m$. Thus, in addition to the upper cutoff $\frac{1}{2}$ on k^2 , we have a lower cutoff:

$$k_{\min}^2 \leq k^2 \leq \frac{1}{2},$$

where

$$k_{\min}^2 \equiv \frac{\lambda}{2(\lambda + \omega^2 \alpha^2)}; \quad \alpha \equiv \frac{1}{\max(|q_a|, |q_b|)}.$$

Note that cn^{-1} is always positive. It monotonically decreases from $\operatorname{cn}^{-1}(-1) = 2K(k)$ to $\operatorname{cn}^{-1}(1) = 0$, with an inflexion point at $(0, K(k))$.

A sample graphical solution of (7) is shown in Figure 2, for $\omega = T = q_a = q_b = 1$. The cases $\lambda = 0.001, 0.5$, and 1 are shown. The curve $\omega T / \sqrt{1-2k^2}$ intersects $\varphi_{\pm}(k^2)$ once, twice, or not at all. Each intersection gives the modulus k for a possible classical path such that $q(t_a) = q_a$ and $q(t_b) = q_b$. There comes a point where each of the curves $\varphi_{\pm}(k^2) + 4NK(k)$ (one for each N) intersects $\omega T / \sqrt{1-2k^2}$ twice for each $N > N_0$. Therefore, there is always a countably infinite number of paths, with a cluster point at $k^2 = \frac{1}{2}$.

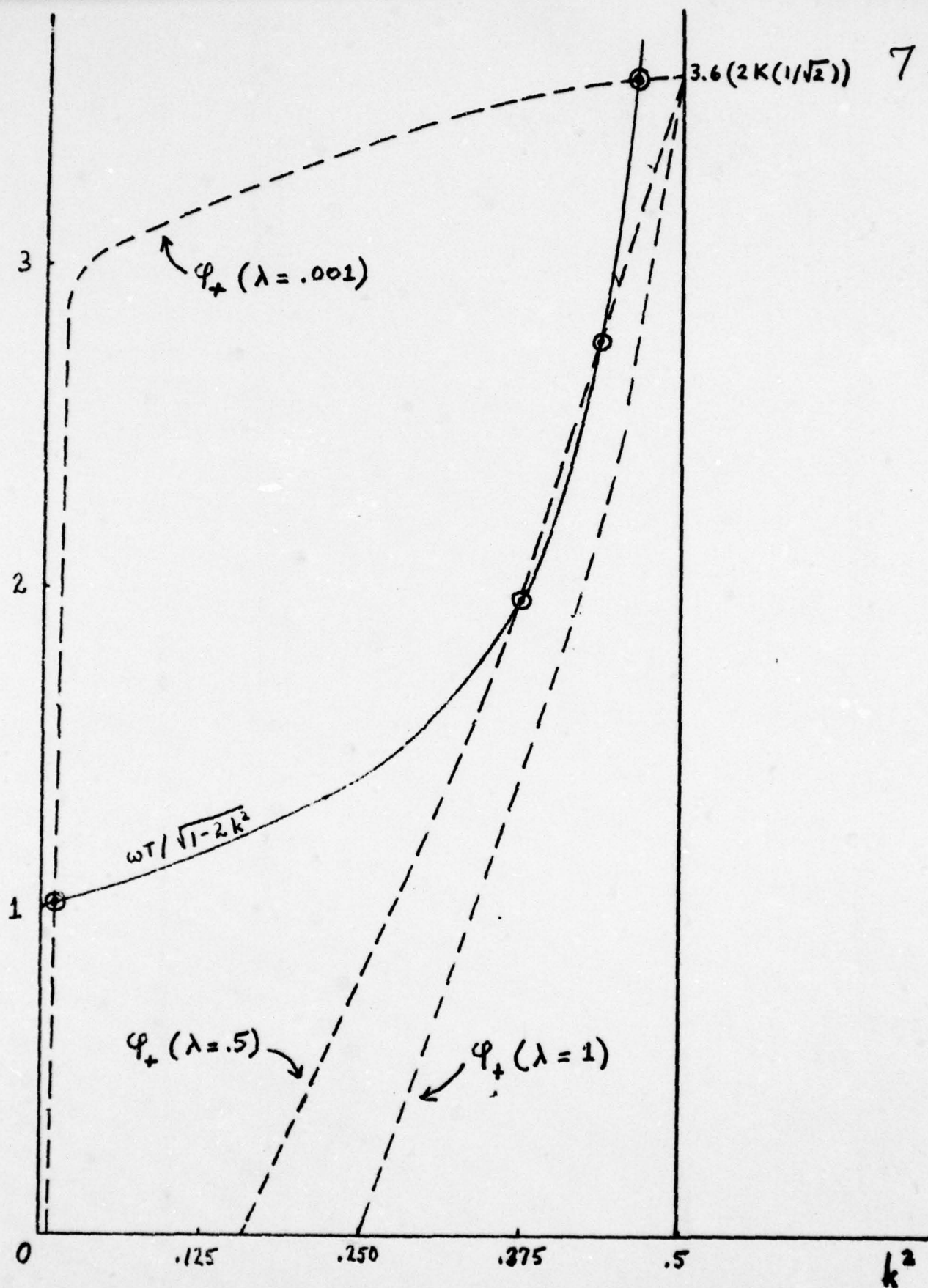


Figure 2. Classical paths for the anharmonic oscillator. Each intersection (circled) gives a value of k which corresponds to a classical solution of the dynamical equation for fixed-endpoint boundary conditions.

The higher the k , the higher the amplitude of the corresponding path (as revealed by Equation 4).

Behavior as $\lambda \rightarrow 0$. We shall be particularly concerned with the behavior of our expressions as λ approaches 0. What happens to the classical solution as $\lambda \rightarrow 0$? For initial boundary conditions, it appears, according to (3), that we retrieve harmonic motion: indeed, as $\lambda \rightarrow 0$, $k \rightarrow 0$, $\Omega \rightarrow \omega$, and $\cos \rightarrow \cos$. However, for other boundary conditions, it appears, according to (4), that we have a $1/\sqrt{\lambda}$ singularity as $\lambda \rightarrow 0$: indeed, for arbitrary values of the constants of integration (say $k^2 = 0.3$ and $t_0 = 2$ seconds), (4) indicates that $q_c(t) \sim 1/\sqrt{\lambda}$ as $\lambda \rightarrow 0$. Is harmonic motion irretrievable then as a limiting case?

The answer is no. The reason is that only physical boundary conditions (such as position and velocity at certain times) are acceptable¹¹. $k^2 = 0.3$ is not a physical boundary condition. When the latter are inserted, k will depend on λ in such a manner as to make at least one classical path $q_c(t)$ reduce to harmonic motion when $\lambda \rightarrow 0$.

In the case of endpoint boundary conditions, (4) shows that the only way that $q_c(t)$ can retain its constant, preassigned values at t_a and t_b is if k^2 goes to 0 as fast as λ . The ratio k^2/λ is then an arbitrary constant A , which may be dependent on ω , and (4) becomes $q_c(t) = A \cos \omega(t-t_0)$, which is harmonic motion. Figure 2 shows that as λ approaches 0 there is always one solution k^2 which also approaches 0. This solution, which we call $q_{co}(t)$, is the lowest-amplitude (or lowest-energy) path, and coincides, when $\lambda = 0$, with the (generally) unique harmonic-oscillator path between the two fixed endpoints. The other paths correspond to values of k which do not go to 0 with λ , and

hence their amplitudes increase without bound as $\lambda \rightarrow 0$. Their graph becomes, in the limit, a set of parallel lines perpendicular to the t -axis, one of which going through t_a and the other through t_b .

Our semiclassical expansion of the propagator will be about this regular path $q_{c0}(t)$. Since all the coefficients will depend, directly or indirectly, on q_{c0} alone, the anharmonic propagator will tend toward the harmonic propagator as the coupling constant tends to 0.

Classical action

The classical action (or action functional evaluated at a classical path) for the anharmonic oscillator is needed for the WKB approximation. It is given by:

$$\begin{aligned} S_c &\equiv \int_{t_a}^{t_b} L(q_c(t), \dot{q}_c(t), t) dt \\ &= \int_{t_a}^{t_b} \left[\frac{1}{2} \dot{q}_c^2(t) - \frac{1}{2} \omega^2 q_c^2(t) - \frac{1}{4} \lambda q_c^4(t) \right] dt. \end{aligned}$$

Using the integrals 312.02 (p. 193), 361.02 (p. 212), 312.04 (p. 193) of Reference 10, and the formula

$$E(u') - E(u) = E(u' - u) - k^2 \operatorname{sn} u \cdot \operatorname{sn} u' \cdot \operatorname{sn}(u' - u), \quad (8)$$

[derived from formulas 116.01 (p. 13) and 123.01 (p. 23) of Reference 10], we obtain the answer:

$$\begin{aligned}
S_c = & \frac{-2\omega^3}{3\lambda\sqrt{1-2k^2}} E\left(\frac{\omega T}{\sqrt{1-2k^2}}\right) + \frac{2\omega^3 k^2}{3\lambda\sqrt{1-2k^2}} \left[\operatorname{sn}(u_a) \operatorname{sn}(u_b) \right. \\
& \cdot \operatorname{sn}\frac{\omega T}{\sqrt{1-2k^2}} + \frac{1}{1-2k^2} \left(\operatorname{sn}(u_a) \operatorname{cn}(u_a) \operatorname{dn}(u_a) - \right. \\
& \left. \left. - \operatorname{sn}(u_b) \operatorname{cn}(u_b) \operatorname{dn}(u_b) \right) \right] + \frac{\omega^4 (1-k^2)(2-3k^2) T}{3\lambda (1-2k^2)^2}, \quad (9)
\end{aligned}$$

where $u_{a/b} \equiv \omega(t_{a/b} - t_0)/\sqrt{1-2k^2}$.

Behavior when $\lambda \rightarrow 0$. Let us look at the behavior of S_c as $\lambda \rightarrow 0$ along the path q_{c0} , where $k^2 \rightarrow 0$ as $\lambda \rightarrow 0$ such that k^2/λ is a constant. Using the fact that $E(u) = u + O(k^2)$, we easily see that S_c is regular at $\lambda=0$, and reduces to the classical action for the harmonic oscillator.

III. THE QUANTUM SYSTEM

The Small-Disturbance Equation

Just as the classical system is dominated by the dynamical (or Euler-Lagrange) equation, the quantum system is dominated by the small-disturbance (or Jacobi) equation. The latter is the equation satisfied by a small variation in the classical path, obtained, for example, by a small change in a constant of integration, such as the total energy or an endpoint. The small-disturbance equation is studied in more detail in Appendix A and in References 1 and 6c. For the anharmonic oscillator, it is:

$$\left[-\frac{d^2}{dt^2} - \omega^2 - 3\lambda q_c^2(t) \right] f(t) = 0. \quad (10)$$

Solutions of the small-disturbance equation

Solutions of the small-disturbance equation can always be generated by differentiating the classical solution with respect to a constant of integration.

This simple procedure was known to Jacobi¹², but it seems to be sometimes forgotten today, as one still finds attempts at solving the equation directly; for example, Sarkar⁸ has undertaken this very difficult task for the anharmonic oscillator (Equation 10).

The functions we will need for the path-integral treatment of the propagator are the Jacobi commutator $J(t, t')$, the Van Vleck - Morette (VVM) function $M(t_a, t_b)$, and the Feynman Green function $G(t, t')$. Their expressions are given below, followed by their definition and derivation.

Jacobi commutator

$$J(t, t') = \frac{(1-2k^2)^{3/2}}{\omega} \operatorname{sn} u \operatorname{sn} u' \operatorname{dn} u \operatorname{dn} u' \cdot$$

$$\left[\frac{-1}{1-2k^2} \left(\frac{\operatorname{cn} u'}{\operatorname{sn} u' \operatorname{dn} u'} - \frac{\operatorname{cn} u}{\operatorname{sn} u \operatorname{dn} u} \right) + \frac{u' - u}{1-2k^2} \right. \quad (11)$$

$$\left. - \frac{E(u' - u)}{k'^2} + \frac{k'^2}{k'^2} \left(\frac{\operatorname{sn} u' \operatorname{cn} u'}{\operatorname{dn} u'} - \frac{\operatorname{sn} u \operatorname{cn} u}{\operatorname{dn} u} \right) + \operatorname{sn} u \operatorname{sn} u' \operatorname{sn}(u' - u) \right],$$

where

$$u \equiv \frac{\omega(t-t_0)}{\sqrt{1-2k^2}}, \quad u' \equiv \frac{\omega(t'-t_0)}{\sqrt{1-2k^2}}, \quad \text{and} \quad k' = 1-k^2;$$

VVM function

$$M(t_a, t_b) = [J(t_a, t_b)]^{-1}; \quad (12)$$

Feynman's Green function

$$G(t, t') = \frac{J(t', t_a) J(t_b, t) Y(t-t') + J(t, t_a) J(t_b, t') Y(t'-t)}{J(t_a, t_b)}. \quad (13)$$

Definitions and derivations

The Jacobi commutator. This function $J(t, t')$ of two variables can be defined as follows: the unique, retarded Green function of the small-disturbance operator, satisfying

$$\left[-\frac{d^2}{dt^2} - \omega^2 - 3\lambda q_c^2(t) \right] G(t, t') = \delta(t - t'), \quad (14)$$

is $G^-(t, t') = J(t, t')Y(t - t')$, where $Y(x) \equiv 1$ for $x > 0$ and 0 otherwise. $J(t, t')$ is antisymmetric and satisfies the small-disturbance equation in both t and t' . It is called the commutator because, as shown in Appendix A, it can be written as a Poisson bracket of position at different times with respect to initial (or final) position and momentum; when the system is quantized, this expression becomes the commutator. For example, for initial boundary conditions, we have:

$$\begin{aligned} J(t, t') &= \frac{\partial q_c(t)}{\partial q_a} \frac{\partial q_c(t')}{\partial p_a} - \frac{\partial q_c(t')}{\partial q_a} \frac{\partial q_c(t)}{\partial p_a} \\ &\equiv \left\{ q_c(t), q_c(t') \right\}_{(q_a, p_a)} \rightarrow \frac{1}{i\hbar} [\tilde{Q}(t), \tilde{Q}(t')]. \end{aligned} \quad (15)$$

For any two convenient constants of integration α_1 and α_2 we can write the commutator as (see proof in Appendix A):

$$J(t, t') = \frac{\frac{\partial q_c(t)}{\partial \alpha_1} \frac{\partial q_c(t')}{\partial \alpha_2} - \frac{\partial q_c(t')}{\partial \alpha_1} \frac{\partial q_c(t)}{\partial \alpha_2}}{\frac{\partial q_c(t_b)}{\partial \alpha_1} \frac{\partial p_c(t_b)}{\partial \alpha_2} - \frac{\partial p_c(t_b)}{\partial \alpha_1} \frac{\partial q_c(t_b)}{\partial \alpha_2}} \quad (16)$$

(or a similar expression with t_b replaced by t_a), where $p_c(t)$ is the classical

momentum (equal to $\dot{q}_c(t)$ for the anharmonic oscillator). We will use this formula with $q_c(t)$ given by (4) and $\alpha_1 = k$, $\alpha_2 = t_0$. The velocity is given by:

$$\dot{q}_c(t) = \frac{-k\omega^2}{1-2k^2} \sqrt{\frac{2}{\lambda}} \operatorname{sn} u \cdot \operatorname{dn} u = -\frac{\partial q_c(t)}{\partial t_0},$$

where u is defined in (11). The formulas for differentiating the elliptic functions with respect to the modulus k are found in Reference 10 (710.51-3, p. 283). Since the argument of the elliptic functions also depends on k , the chain rule must be used to evaluate $\partial q_c(t)/\partial k$ and $\partial \dot{q}_c(t_b)/\partial k$. We obtain:

$$\begin{aligned} \frac{\partial q_c(t)}{\partial k} = & \omega \sqrt{\frac{2}{\lambda}} \frac{\operatorname{cn} u}{(1-2k^2)^{3/2}} - \sqrt{\frac{2k^2\omega^2}{\lambda(1-2k^2)}} \operatorname{sn} u \cdot \operatorname{dn} u \left\{ \frac{2k\omega(t-t_0)}{(1-2k^2)^{3/2}} \right. \\ & \left. + (1/kk'^2) [-E(u) + k'^2 u + k^2 \operatorname{sn} u \cdot \operatorname{cn} u / \operatorname{dn} u] \right\}. \end{aligned}$$

The denominator in (16) is calculated to be:

$$\frac{\partial q_b}{\partial k} \frac{\partial \dot{q}_c(t_b)}{\partial t_0} - \frac{\partial \dot{q}_c(t_b)}{\partial k} \frac{\partial q_b}{\partial t_0} = \frac{2\omega^4 k}{\lambda(1-2k^2)^3}.$$

These formulas, along with (8), lead us to the stated expression (11) for $J(t, t')$. We see that for $q_c = q_{c0}$, i.e. when k^2 goes to 0 with λ , we have $E(u) \rightarrow u$, $\operatorname{dn} u \rightarrow 1$, $\operatorname{sn} u \rightarrow \sin u$, $\operatorname{cn} u \rightarrow \cos u$, $u \rightarrow \omega(t-t_0)$, and $J(t, t') \rightarrow \omega^{-1} \sin \omega(t'-t)$, which is the harmonic-oscillator commutator function.

The VVM function. The WKB approximation to the propagator is given by the well-known formula:

$$K_{WKB} = (M/2\pi i \hbar)^{1/2} \exp(iS_c/\hbar), \quad (17)$$

where

$$M \equiv - \frac{\partial^2 S_c}{\partial q_a \partial q_b} = - \frac{\partial \dot{q}_c(t_b)}{\partial q_a} \quad (18)$$

is the Van Vleck - Morette function. The second expression for M , which will be used in the evaluation, uses the fact that $\partial S_c / \partial q_b = p_c(t_b) = \dot{q}_c(t_b)$.¹³ Therefore, to get M in terms of k and t_0 we must use the chain rule:

$$M = - \frac{\partial \dot{q}_c(t_b)}{\partial k} \frac{\partial k}{\partial q_a} - \frac{\partial \dot{q}_c(t_b)}{\partial t_0} \frac{\partial t_0}{\partial q_a}. \quad (19)$$

In order to calculate M , we must express $\partial k / \partial q_a$ and $\partial t_0 / \partial q_a$ in terms of $\partial q_a / \partial k$, $\partial q_a / \partial t_0$, etc. Since we must have

$$\begin{pmatrix} k_1 & k_2 \\ k_3 & k_4 \end{pmatrix} \begin{pmatrix} u_1 & u_2 \\ u_3 & u_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

where

$$k_1 \equiv \frac{\partial q_a}{\partial k}$$

$$k_2 \equiv \frac{\partial q_a}{\partial t_0}$$

$$u_1 \equiv \frac{\partial k}{\partial q_a}$$

$$u_2 \equiv \frac{\partial k}{\partial q_b}$$

$$k_3 \equiv \frac{\partial q_b}{\partial k}$$

$$k_4 \equiv \frac{\partial q_b}{\partial t_0}$$

$$u_3 \equiv \frac{\partial t_0}{\partial q_a}$$

$$u_4 \equiv \frac{\partial t_0}{\partial q_b},$$

we can easily solve for the u 's in terms of the k 's, to get

$$u_1 = \frac{k_4}{\mathcal{D}}, \quad u_2 = -\frac{k_2}{\mathcal{D}}, \quad u_3 = -\frac{k_3}{\mathcal{D}}, \quad u_4 = \frac{k_1}{\mathcal{D}},$$

where $\mathcal{Q} \equiv k_1 k_4 - k_2 k_3$. Substituting this result in (19), and comparing with (16), we see that we get the value of M stated in (12), namely $M = [J(t_a, t_b)]^{-1}$.

Feynman's Green function. Feynman's Green function $G(t, t')$, satisfying (14), is the unique Green function of the small-disturbance operator which vanishes at both endpoints. It is important for our treatment because it is the covariance of the Gaussian measure used to express the propagator as a path integral. As was stated before (and proved in Appendix A), $G^-(t, t') \equiv J(t, t')Y(t-t')$, with J as in (16), satisfies (14). The function

$$G(t, t') \equiv J(t, t')Y(t-t') + \frac{J(t, t_a)J(t_b, t')}{J(t_a, t_b)}$$

is also a Green function, since the addition to $G^-(t, t')$ is a homogeneous solution of the small-disturbance equation in t and t' . Further, $G(t_a, t') = G(t_b, t') = 0$. Therefore, $G(t, t')$ is Feynman's Green function. To put it in the form given in (13) requires use of the identity

$$J(t, t') = \frac{J(t', t_a)J(t_b, t) - J(t, t_a)J(t_b, t')}{J(t_a, t_b)},$$

easily proved by using (16).

IV. WKB EXPANSION OF THE PROPAGATOR BY PATH INTEGRALS

Arbitrary Potential

The framework for a WKB expansion of the propagator by phase-space path integrals without limiting procedure was set in an earlier paper¹⁴ and will be only briefly summarized here. For a simple Hamiltonian of the form $p^2/2m + V(q, t)$ considered here, the phase-space path integral becomes a configuration-space path

integral, since the momentum-dependent terms are rolled into the measure and only position-dependent terms remain to be path-integrated. The first step is to expand the classical action functional about the classical path $q_c(t)$:

$$S[q] \equiv S[q_c + x] = S_c + \frac{1}{2} \int_T [\dot{x}^2(t) - V''(t)x^2(t)] dt - \sum_{n=3}^{\infty} \frac{1}{n!} \int_T V^{(n)}(t) x^n(t) dt,$$

where

$$V^{(n)}(t) \equiv \left[\partial^n V(q, t) / \partial q^n \right]_{q=q_c},$$

$T \equiv [t_a, t_b]$, and $x \in \mathcal{C}_c$, the space of paths such that $x(t_a) = x(t_b) = 0$. The classical action S_c becomes part of the WKB approximation, K_{WKB} , and the quadratic terms are rolled into the Gaussian measure, leaving the sum term for path integration. The result is:

$$K = K_{\text{WKB}} \int_{\mathcal{C}_c} dw_0(x) \exp \left\{ -\frac{i}{\hbar} \sum_{n=3}^{\infty} \int_T V^{(n)}(t) \frac{x^n(t)}{n!} dt \right\}, \quad (20)$$

where the measure w_0 is defined by its Fourier transform:

$$\mathcal{F}w_0(\mu) \equiv \exp \left[-\frac{i\hbar}{2} \iint_{T \times T} G(t, t') d\mu(t) d\mu(t') \right],$$

$G(t, t')$ being Feynman's Green function defined earlier and μ being a bounded measure on the time-interval T . K_{WKB} is given by (17). The exponential in (20) can be expanded to yield:

$$K = K_{\text{WKB}} \left[1 + \sum_{j=1}^{\infty} \frac{1}{j!} \left(\frac{-i}{\hbar} \right)^j \sum_{n_1=3}^{\infty} \dots \sum_{n_j=3}^{\infty} \int_T \frac{dt_1 \dots dt_j}{n_1! \dots n_j!} \right. \\ \left. \times V^{(n_1)}(t_1) \dots V^{(n_j)}(t_j) \int_{\mathcal{C}_0} x^{n_1}(t_1) \dots x^{n_j}(t_j) dw_0(x) \right]. \quad (21)$$

To evaluate the path integral, we need the moments formula [see, e.g., Reference 15]:

$$\int_{\mathcal{C}_0} x(t_1) x(t_2) \dots x(t_n) dw_0(x) = \begin{cases} 0 & \text{if } n \text{ is odd} \\ (i\hbar)^m \sum' G(t_{i_1}, t_{i_2}) G(t_{i_3}, t_{i_4}) \dots \\ \dots G(t_{i_{2m-1}}, t_{i_{2m}}) & \text{if } n=2m \text{ is even,} \end{cases} \quad (22)$$

where \sum' denotes the sum over all different combinations of different indices i_j , with $\{i_1, i_2, \dots, i_n\} \equiv \{1, 2, \dots, n\}$. There are $(2m-1)!! \equiv (2m-1)(2m-3)\dots$ 5.3.1 terms in all for $n = 2m$.¹⁶

Thus, we see that \hbar comes in the expansion with power $\frac{1}{2}(n_1 + \dots + n_j) - j$, which is always a positive integer, since each n_i is at least 3. This proves that (21) is indeed an expansion in powers of \hbar , and we can write:

$$K = K_{\text{WKB}} (1 + \hbar K_1 + \hbar^2 K_2 + \dots), \quad (23)$$

where the K_i s are ordinary finite-dimensional integrals over the time-interval T . Polynomial potentials are best suited for this scheme, since the expansion of the action terminates at some finite n . However, it is important to note that regardless of the potential each term in the WKB expansion (coefficient of \hbar^k) is always a terminating series. For example, inspection of (21) shows that the first (post-WKB) term is, for arbitrary potential:

$$\hbar K_1 = \left(-\frac{i}{\hbar}\right) \int_T \frac{dt}{4!} V^{(4)}(t) \int_{\mathcal{C}_0} x^4(t) d\omega_0(x) \quad (24)$$

$$+ \frac{1}{2} \left(-\frac{i}{\hbar}\right)^2 \int_{T^2} \frac{dt}{3!} \frac{ds}{3!} V^{(3)}(t) V^{(3)}(s) \int_{\mathcal{C}_0} x^3(t) x^3(s) d\omega_0(x),$$

and the moments formula gives:

$$K_1 = -\frac{i}{\hbar} \int_T V^{(4)}(t) G^2(t, t) dt \quad (25)$$

$$+ \frac{i}{24} \int_{T^2} V^{(3)}(t) V^{(3)}(s) [3 G(t, t) G(t, s) G(s, s) + 2 G^3(t, s)] dt ds.$$

Let us study the structure of the coefficients K_j . In general, the $j = 1$ term in (19) is:

$$\left(-\frac{i}{\hbar}\right) \sum_{n=3}^{\infty} \int_T \frac{dt}{n!} V^{(n)}(t) \int_{\mathcal{C}_0} x^n(t) d\omega_0(x) \quad (26)$$

$$= \sum_{m=2}^{\infty} \frac{(1+\hbar)^{m-1}}{m! 2^m} \int_T V^{(2m)}(t) G^m(t, t) dt.$$

For arbitrary potentials, this is an infinite series in \hbar with no constant term. Similarly, we find that:

- In the series for $j = 2$, the $n_1 = n_2 = 3$ term is the term proportional to \hbar , and the three terms $n_1 = n_2 = 4$; $n_1 = 3, n_2 = 5$; and $n_1 = 5, n_2 = 3$ are the one proportional to \hbar^2 . All the subsequent j series start out with \hbar^k for $k \geq 2$.
- In the series for $j = 3$, the three terms $n_1 = n_2 = 3, n_3 = 4$; $n_1 = 4, n_2 = n_3 = 3$; and $n_1 = n_3 = 3, n_2 = 4$ are the only ones proportional to \hbar^2 , and the $n_1 = n_2 = n_3 = 4$ term is the only one proportional to \hbar^3 .
- In the series for $j = 4$, the term $n_1 = n_2 = n_3 = n_4 = 3$ is the only one proportional to \hbar^2 .
- The series for $j = 5$ starts out with the \hbar^3 term.

Thus, we can write the term proportional to \hbar^2 in the expansion:

$$\begin{aligned}
\hbar^2 K_2 = & \frac{-\hbar^2}{48} \int_T V^{(6)}(t) G^3(t, t) dt \\
& - \frac{1}{2\hbar^2} \int_{T^2} \frac{dt_1}{4!} \frac{dt_2}{4!} V^{(4)}(t_1) V^{(4)}(t_2) \int_{\mathcal{C}_0} x^4(t_1) x^4(t_2) \cdot d\omega_0(x) \\
& - \frac{1}{2\hbar^2} \int_{T^2} \frac{dt_1}{3!} \frac{dt_2}{5!} V^{(3)}(t_1) V^{(5)}(t_2) \int_{\mathcal{C}_0} x^3(t_1) x^5(t_2) d\omega_0(x) \\
& + \frac{i}{6\hbar^3} \int_{T^3} \frac{dt_1}{3!} \frac{dt_2}{3!} \frac{dt_3}{4!} V^{(3)}(t_1) V^{(3)}(t_2) V^{(4)}(t_3) \cdot \int_{\mathcal{C}_0} x^3(t_1) x^3(t_2) x^4(t_3) d\omega_0(x) \\
& + \frac{1}{4! \hbar^4} \int_{T^4} \frac{dt_1 \dots dt_4}{(3!)^4} V^{(3)}(t_1) V^{(3)}(t_2) V^{(3)}(t_3) V^{(3)}(t_4) \cdot \int_{\mathcal{C}_0} x^3(t_1) x^3(t_2) x^3(t_3) x^3(t_4) d\omega_0(x),
\end{aligned} \tag{27}$$

and the moments formula (22) gives the value of the path integrals in terms of Feynman's Green function and the classical path.

Application to the Anharmonic Potential

The anharmonic oscillator potential, given by (1), is $V(q) = m\omega^2 q^2/2 + \lambda q^4/4$. The first-order correction to the WKB approximation is then given by (25):

$$K_1 = \frac{-3\lambda i}{4} \int_T G^2(t,t) dt + \frac{3\lambda^2 i}{2} \int_T dt \int_T ds q_c(t) q_c(s) \times [3 G(t,t) G(t,s) G(s,s) + 2 G^3(t,s)], \quad (28)$$

where $G(t,t')$ is given explicitly by (13) with J given by (11) and $q_c(t)$ by (4). The resulting integrals over the elliptic functions are all well-known and of the type tabulated in Reference 10. Higher-order corrections can be generated at will, although they generally involve a large number of integrals. The WKB approximation is given by (17), with the classical action S_c given by (9) and the VVM function M given by (12), with J in (11). Therefore, every function entering the semiclassical expansion of the anharmonic oscillator propagator has been explicitly calculated, and the definite integrals giving the coefficients of the expansion have been explicitly exhibited. It is pointed out, again, that this treatment is nonperturbative, since the functions involved in the terms of the expansion, for example q_c and G in (28), depend implicitly on λ . This example illustrates the power of path integration without limiting procedure.

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FOOTNOTES

1. This paper is based in part on the author's Ph.D. dissertation, "An Investigation of the Feynman Path Integral Formulation of Quantum Mechanics", The University of Texas at Austin, Austin, Texas, August 1975.
2. J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, Phys. Lett. 30B(1969), 656-8, and Barry Simon, Ann. of Phys. 58 (1970), 76-136.
3. Indeed, the dynamical equation for the $\lambda \varphi^4$ self-interaction, $(\square - m^2)\varphi - \lambda \varphi^3 = 0$, can be readily reduced to the dynamical equation for the one-dimensional anharmonic oscillator, namely $\bar{\varphi}'' - m^2 \bar{\varphi}/K^2 - \lambda \bar{\varphi}^3/K^2 = 0$, where $\varphi(x_1, x_2, x_3, x_4) \equiv \bar{\varphi}(K \cdot x)$, K being an arbitrary four-vector (plane-wave solution). The elliptic functions which are solutions of this equation are periodic, and admit of a restricted superposition principle, rare for non-linear equations: if an elliptic cosine (cn) with a certain modulus k_1 is a solution, and if an elliptic sine (sn) with another modulus k_2 is also a solution, then the linear combination $(cn + i sn)$ is also a solution, but the common modulus k_3 is different from k_1 and k_2 (cf. Gérard Pétiau, Cahiers de Physique 14 (1960), 1-24, and D. F. Kurdgelaidzé, Cahiers de Physique, No. 128 (1961), 149-57).
4. Carl M. Bender and Tai Tsun Wu, Phys. Rev. Lett. 21 (1968), 406-9; Phys. Rev. 184 (1969), 1231-60; Phys. Rev. Lett. 27 (1971), 461-5; Phys. Rev. D7 (1973), 1620-36.

5. P. M. Mathews and K. Eswaran, *Lett. Nuov. Cim.* 5 (1972), 15-8.
6. C. DeWitt-Morette, (a) *Comm. Math. Phys.* 28 (1972), 47-67; (b) 37 (1974), 63-81; (c) *Ann. of Phys.* 97 (1976), 367-99; (d) (with A. Maheshwari and B. Nelson), to appear in *Phys. Rep.*
7. C. S. Lam, *Nuov. Cim. Serie X*, 47 (1967), 451-69; 50 (1967), 504-10.
8. S. Sarkar, *Phys. Rev.* D8 (1973), 1060-7.
9. P.M. Mathews and M. S. Seshadri, *Int. Jour. of Theor. Phys.* 13 (1975), 279-88.
10. Paul F. Byrd and Morris D. Friedman, Handbook of Elliptic Integrals for Engineers and Physicists. Berlin: Springer-Verlag, 1954.
11. We can better understand this question of physical boundary conditions from the simpler example of a particle in free fall with friction taken into account. The dynamical equation is $\ddot{x} = -(g + k\dot{x})$, with solution $x(t) = -gt/k + Ak^{-2}e^{-kt} + B$, where A and B are constants of integration. When $k \rightarrow 0$, we expect to retrieve free fall: $x(t) = -gt^2/2 + v_0 t + x_0$. Instead, we find a "singularity" at $k = 0$ if A and B are numerically specified. However, numerical specification of A and B does not constitute physical boundary conditions. Physical boundary conditions, such as $x(t_0) = x_0$ and $\dot{x}(t_0) = v_0$, always make A and B depend on k in such a manner as to make the solution, [namely, in this case, $x(t) = x_0 - gt/k + (g + v_0 k)(1 - e^{-kt})/k^2$], reduce properly when $k \rightarrow 0$.

12. Jacobi, "On the theory of the calculus of variations and of differential equations", Crelle's Mathematical Journal 17 (1837), referred to in Bolza's Calculus of Variations, p. 56.

13. This relation and similar ones can be simply derived as follows. For any Lagrangian L in n dimensions and $u \equiv t_a, t_b, q_a$, or q_b , we have $\partial S_c / \partial u$
 $= (\partial / \partial u) \int_{t_a}^{t_b} L(q_c, \dot{q}_c, t) dt = (p_c)_i(t_b) [\partial q_c^i(t) / \partial u]_{t=t_b} - (p_c)_i(t_a)$
 $\times [\partial q_c^i(t) / \partial u]_{t=t_a} + \epsilon L(u),$

where $\epsilon = 0$ for $u = q_a$ or $u = q_b$, 1 for $u = t_b$ and -1 for $u = t_a$, since

$(p_c)_i(t) \equiv [\partial L / \partial \dot{q}^i]_{q=q_c}$. Given that the classical
 Hamiltonian is $H_c(p_c, q_c, t) \equiv (p_c)_i(\dot{q}_c^i)^i - L(q_c, \dot{q}_c, t)$,

this gives the following 4 relations of Hamilton-Jacobi theory:

$$\begin{aligned} \partial S_c / \partial q_a^i &= -(p_c)_i(t_a) & \partial S_c / \partial t_a &= H_c(-\partial S_c / \partial q_a, q_a, t_a) \\ \partial S_c / \partial q_b^i &= (p_c)_i(t_b) & \partial S_c / \partial t_b &= -H_c(\partial S_c / \partial q_b, q_b, t_b). \end{aligned}$$

14. Maurice M. Mizrahi, J. Math. Phys. 19 (1978), 298-307.

15. Maurice M. Mizrahi, J. Math. Phys. 17 (1976), 566-75.

16. Among the specific moments needed are the following:

$$\begin{aligned} \text{a) } \int_{\mathcal{C}} x^{2n}(t) dW_t(x) &= (2n)! \hbar^n i^n G^n(t, t) / 2^n n! \\ \text{b) } \int_{\mathcal{C}} x^2(t) x^2(t') dW_t(x) &= -\hbar^2 [G(t, t) G(t', t') + 2G^2(t, t')] \end{aligned}$$

$$c) \int_{\mathcal{C}_0} x^3(t) x^3(t') dw_0(x) = -i\hbar^3 [9G(t,t)G(t,t')G(t',t') + 6G^3(t,t')]$$

$$d) \int_{\mathcal{C}_0} x^2(t) x^4(t') dw_0(x) = -i\hbar^3 [12G^2(t,t')G(t',t') + 3G(t,t)G^2(t',t')]$$

$$e) \int_{\mathcal{C}_0} x^4(t) x^4(t') dw_0(x) = \hbar^4 [9G^2(t,t)G^2(t',t') + 24G^4(t,t') + 72 G(t,t)G(t',t')G^2(t,t')]$$

For higher moments, we need a compressed notation. We write:

$$12 \hbar^3 G^2(t_1, t_2) G(t_2, t_2) \equiv 12 (12)^2 (22).$$

Then,

$$\begin{aligned} f) \int_{\mathcal{C}_0} x^3(t_1) x^3(t_2) x^4(t_3) dw_0(x) = & 27 (11) (12) (22) (33)^2 \\ & + 18 (12)^3 (33)^2 + 72 (31)^3 (32) (22) \\ & + 72 (31) (32)^3 (11) + 108 (33) (31) (32) (11) (22) \\ & + 108 (33) (32)^2 (11) (12) + 108 (33) (31)^2 (22) (21) \\ & + 216 (31)^2 (32)^2 (12) + 216 (33) (31) (32) (12)^2. \end{aligned}$$

There are $(3+3+4 - 1)!! = 9 \times 7 \times 5 \times 3 = 945$ terms in all .

17. J. Milnor, Morse Theory, Based on lecture notes by M. Spivak and R. Wells. Princeton University Press, 1969. Annals of Mathematics Studies, No. 51.

18. Bryce S. DeWitt, Dynamical Theory of Groups and Fields. New York: Gordon and Breach, 1965.

19. C. DeWitt-Morette, in Long-Term Predictions in Dynamics, edited by V. Szebehely and B. D. Tapley, Dordrecht: D. Reidel, 1976, pp. 57-65; also pp. 67-70 (with Pete Tschumi).

APPENDIX A -- THE SMALL-DISTURBANCE EQUATION

This appendix will derive and generalize some results used in the text on the equation of small disturbances. The latter, resulting from the second variation of the action functional, is satisfied by the variation in a classical path resulting from a small change in the boundary conditions. For example, let $S[q] = S[\bar{\beta}(u)]$ be an action functional. Each path $q \equiv \bar{\beta}(u)$ is characterized by a parameter u : $q(t) = \bar{\beta}(u)(t) \equiv \beta(u, t)$. If the set $\{\bar{\beta}(u)\}$ is a set of classical paths $\{q_c(u)\}$ labeled by a parameter u (say a constant of integration), then $S'[\bar{\beta}(u)] = 0$ by definition of $\bar{\beta}(u)$. If we differentiate with respect to u , we get:

$$S''[\bar{\beta}(u)] \frac{\partial \bar{\beta}(u)}{\partial u} = 0. \quad (A1)$$

This is the small-disturbance equation with its explicit solution in terms of the classical path: $S''[\bar{\beta}(u)]$ (second functional derivative of the action evaluated at the classical path) yields the small-disturbance operator; $\partial \bar{\beta}(u)/\partial u$ is its explicit solution, called a Jacobi field along the classical path $\bar{\beta}(u)$. Thus, the derivative of a classical solution with respect to a constant of integration is a solution of the small-disturbance equation. Note that if S is derived from a Lagrangian which does not contain the time explicitly, and we take the time derivative of the differential equations resulting from $S'[\bar{\beta}(u)] = 0$, we find that the classical velocity $\partial \bar{\beta}(u)(t)/\partial t$ is also a solution of (A1).

This method of "variation through geodesics" was studied extensively by J. Milnor¹⁷. The approach was generalized by C. DeWitt-Morette^{6c} for arbitrary action functionals, and independently by the author¹ for Lagrangian actions. This method of generating solutions of (A1) was known to Jacobi¹².

Lagrangian Action

Let us consider the Lagrangian action in n dimensions as a specific example:

$$S[q] \equiv \int_{t_a}^{t_b} L(q(t), \dot{q}(t), t) dt.$$

One can show by straightforward differentiation with respect to u that the linear mapping $S'[\bar{\beta}(u)]$ maps x into

$$S'[\bar{\beta}(u)]x = \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) \right]_{q=\bar{\beta}(u)}(t) x^i(t) dt \quad (A2)$$

if $x(t_b) = x(t_a) = 0$ and there are no discontinuities in the momentum $\partial L / \partial \dot{q}^i$. Differentiating once more with respect to u yields:

$$S''[\bar{\beta}(u)] \frac{\partial \bar{\beta}(u)}{\partial u} x = \int_{t_a}^{t_b} \left\{ A_{ij}(t) + B_{ij}(t) \frac{\partial}{\partial t} + C_{ij}(t) \frac{\partial^2}{\partial t^2} \right\} \frac{\partial \beta^j(u, t)}{\partial u} x^i(t) dt, \quad (A3)$$

where

$$(a) A_{ij}(t) \equiv \frac{\partial^2 L}{\partial q^i \partial q^j} - \frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} \right)$$

$$(b) B_{ij}(t) \equiv \frac{\partial^2 L}{\partial q^i \partial \dot{q}^j} - \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} - \frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \right)$$

$$(c) C_{ij}(t) \equiv - \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}. \quad (A4)$$

Note that the above matrices satisfy the relations:

$$\begin{aligned}\tilde{C} &= C & (B - \dot{C})\tilde{} &= -(B - \dot{C}) \\ B + \tilde{B} &= 2\dot{C} & A - \tilde{A} &= \dot{B} - \ddot{C} = \frac{1}{2}(\dot{B} - \ddot{B}).\end{aligned}$$

We assume that $C(t)$, the Jacobian of the transformation from the \dot{q} 's to the p 's, never vanishes, so that a canonical formalism exists.

If $\bar{\beta}(u)$ is a family of classical paths q_c , then both sides of (A2) and (A3) are zero for all $x(t)$:

$$\left[\frac{\partial L}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) \right]_{q=q_c} = 0 \quad (A5)$$

$$\left[A_{ij}(t) + B_{ij}(t) \frac{d}{dt} + C_{ij}(t) \frac{d^2}{dt^2} \right]_{q=q_c} f^j(t) = 0. \quad (A6)$$

The first equation is the familiar Euler-Lagrange equation, yielding the classical solutions $q_c(t, u)$ where u is any of the $2n$ constants of integration, or any other parameter (e.g. t_a or t_b).

The second equation is the small-disturbance equation, and the bracketed second-order linear differential operator is the (Hermitian) small-disturbance operator. It is solved by $\partial q_c(t, u) / \partial u$.

Attempts at solving (A6) by "frontal assault" are sometimes found in the literature (see, e.g., Reference 8), and usually yield only approximate solutions, if any at all.

A convenient set of solutions is obtained by using endpoint boundary conditions:

$$q_c^i(t_a) = q_a^i \quad q_c^i(t_b) = q_b^i.$$

Thus, for any fixed $\{i, i'\} = \{1, 2, \dots, n\}$, the two sets:

$$f_{(i)}^j(t) \equiv \frac{\partial q_c^j(t)}{\partial q_a^i} \quad g_{(i')}^j(t) \equiv \frac{\partial q_c^j(t)}{\partial q_b^{i'}}$$

are sets of solutions of (A6) satisfying the obvious boundary conditions:

$$\begin{aligned} f_{(i)}^j(t_a) &= \delta_{ij} & g_{(i)}^j(t_a) &= 0 \\ f_{(i)}^j(t_b) &= 0 & g_{(i)}^j(t_b) &= \delta_{ij} \end{aligned}$$

We can use these solutions as building blocks for other solutions, which can usually be written as linear combinations of them.

Two other sets of solutions can be obtained by differentiating $q_c(t)$ with respect to t_a or t_b :

$$h^j(t) \equiv \frac{\partial q_c^j(t)}{\partial t_a} \quad k^j(t) \equiv \frac{\partial q_c^j(t)}{\partial t_b}$$

They satisfy the boundary conditions:

$$\begin{aligned} h^j(t_a) &= -\dot{q}_c^j(t_a) & k^j(t_a) &= 0 \\ h^j(t_b) &= 0 & k^j(t_b) &= -\dot{q}_c^j(t_b) \end{aligned}$$

Proof. The second and third are obvious since the operations, say, " $\partial/\partial t_a$ " and "evaluate at t_b " commute. The first and fourth are more subtle. The first is derived as follows:

$$\begin{aligned} h^j(t_a) &= -[h^j(t_b) - h^j(t_a)] = -\int_{t_a}^{t_b} \frac{\partial \dot{q}_c^j(t)}{\partial t_a} dt \\ &= -\frac{\partial}{\partial t_a} \int_{t_a}^{t_b} \dot{q}_c^j(t) dt - \dot{q}_c^j(t_a) \\ &= -\frac{\partial}{\partial t_a} (q_b^j - q_a^j) - \dot{q}_c^j(t_a) = -\dot{q}_c^j(t_a) \blacksquare \end{aligned}$$

The fourth relation is derived in a similar manner.

Theorem. Let $x(t)$ and $y(t)$ be two solutions of the small disturbance equation (A6) in one dimension. Their Wronskian depends on t only, through $C(t)$:

$$W(t) \equiv \dot{x}(t)y(t) - x(t)\dot{y}(t) = \alpha C(t_a) C^{-1}(t), \quad (A7)$$

where α is a constant, and it is assumed that $C(t)$ never vanishes.

If $\alpha \neq 0$, x and y are linearly independent.

Proof.

$$\begin{aligned} \dot{W} &= \ddot{x}y - \ddot{y}x = -C^{-1}(A_x + B\dot{x})y + C^{-1}(A_y + B\dot{y})x \\ &= -BC^{-1}(\dot{x}y - \dot{y}x) = -BC^{-1}W \\ \implies W(t) &= \alpha \exp \left[-\int_{t_a}^t B(s) C^{-1}(s) ds \right]. \end{aligned}$$

However, we can see from (A4) that $B = \dot{C}$ in one dimension, and the result follows.

Green Functions

We now study the Green functions $G^{jk}(t, t')$ of the small-disturbance operator, which satisfy:

$$\left[A_{ij}(t) + B_{ij}(t) \frac{\partial}{\partial t} + C_{ij}(t) \frac{\partial^2}{\partial t^2} \right] G^{jk}(t, t') = \delta_i^k \delta(t - t'), \quad (A8)$$

where A, B, and C are given by (A4) for $q = q_c$. We restrict ourselves to one dimension.

Theorem

The advanced and retarded Green functions are unique and are given by

$$G^-(t, t') = G^+(t', t) = J(t, t') Y(t - t') \quad (A9)$$

where $J(t, t')$ is the Jacobi commutator:

$$J(t, t') = \frac{\frac{\partial q_c(t)}{\partial \alpha_1} \frac{\partial q_c(t')}{\partial \alpha_2} - \frac{\partial q_c(t')}{\partial \alpha_1} \frac{\partial q_c(t)}{\partial \alpha_2}}{\frac{\partial q_c(t_b)}{\partial \alpha_1} \frac{\partial p_c(t_b)}{\partial \alpha_2} - \frac{\partial p_c(t_b)}{\partial \alpha_1} \frac{\partial q_c(t_b)}{\partial \alpha_2}}, \quad (A10)$$

α_1 and α_2 being any two constants of integration. t_b in the denominator can be replaced by t_a .

Proof. We look for the most general Green function of the form $G^-(t, t') = f(t, t') Y(t - t')$. Upon differentiation, and use of the fact that $x \delta'(x) = -\delta(x)$, we have:

$$\frac{\partial G^-}{\partial t} = f_{,1}(t, t') \gamma(t-t') + f(t, t') \delta(t-t')$$

$$\frac{\partial^2 G^-}{\partial t^2} = f_{,11}(t, t') \gamma(t-t') + 2f_{,1}(t, t') \delta(t-t') - f(t, t') \frac{\delta(t-t')}{t-t'}$$

$$\begin{aligned} D_t G^- &\equiv \left[A(t) + B(t) \frac{\partial}{\partial t} + C(t) \frac{\partial^2}{\partial t^2} \right] G^- \\ &= \gamma(t-t') D_t f(t, t') + \delta(t-t') \left[B(t) + 2C(t) \frac{\partial}{\partial t} - \frac{C(t)}{t-t'} \right] f(t, t'), \end{aligned}$$

where $f_{,1}(t, t')$ denotes the derivative with respect to the first argument, evaluated at (t, t') .

Thus, G^- is a Green function if $D_t f(t, t') = 0$, i.e. if $f(t, t')$ is a homogeneous solution in t , and if the coefficient of the delta function at $t = t'$ is 1. If we expand about $t = t'$:

$$f(t, t') = f(t, t) + (t-t') f_{,1}(t, t) + \frac{1}{2} (t-t')^2 f_{,11}(t, t) + \dots,$$

the second condition gives the boundary conditions on f :

$$\begin{cases} f(t, t) = 0, \text{ since } C(t) \neq 0 \\ f_{,1}(t, t) = C^{-1}(t). \end{cases}$$

If $f(t, t')$ is a solution in t , then we can write

$$f(t, t') = \beta(t') x(t) + \gamma(t') y(t),$$

where x and y are two linearly independent solutions. If we insert

the boundary conditions, and remember (A7), which indicates that $\dot{x}y - x\dot{y} = \alpha C(t_a)C^{-1}(t)$, we have:

$$f(t, t') = \frac{x(t)y(t') - x(t')y(t)}{C(t_a)[y(t_a)\dot{x}(t_a) - \dot{y}(t_a)x(t_a)]}. \quad (A11)$$

Let us choose $x(t) = \partial q_c(t) / \partial \alpha_1$ and $y(t) = \partial q_c(t) / \partial \alpha_2$. By definition of $C(t)$, $C(t_a) \equiv -\partial^2 L / \partial \dot{q}_c^2(t_a) = -\partial p_c(t_a) / \partial \dot{q}_c(t_a)$, so $-C(t_a) \partial \dot{q}_c(t_a) / \partial \alpha_1 = \partial p_c(t_a) / \partial \alpha_1$. Inserting this in (A11) we see that $f(t, t')$ is given by $J(t, t')$ in (A10). Note that our $J(t, t')$ is what Bryce DeWitt¹⁸ calls \tilde{G} (he defines \tilde{G} by $G^+ - G^-$, but since his Green functions are the negative of ours, $\tilde{G} = J$).

The greatest simplification in $J(t, t')$ as expressed in (A10) occurs when the constants of integration are initial (or final) position and momentum, for example $\alpha_1 = q_c(t_a) = q_a$, $\alpha_2 = p_c(t_a) = p_a$. The denominator is then equal to 1, and

$$J(t, t') = \frac{\partial q_c(t)}{\partial q_a} \frac{\partial q_c(t')}{\partial p_a} - \frac{\partial q_c(t')}{\partial q_a} \frac{\partial q_c(t)}{\partial p_a} \equiv \left\{ q_c(t), q_c(t') \right\}_{(q_a, p_a)}.$$

This Poisson bracket becomes the commutator $[\hat{Q}(t), \hat{Q}(t')] / i\hbar$ when the system is quantized, whence the name of the function.

Feynman's Green function, which vanishes at t_a and t_b , can be built from G^- and G^+ as follows:

$$\begin{aligned} G(t, t') &= G^-(t, t') + J(t, t_a) J(t_b, t') / J(t_a, t_b) \\ &= G^+(t, t') + J(t, t_b) J(t_a, t') / J(t_a, t_b). \end{aligned} \quad (A12)$$

Indeed, it is readily apparent that the additions to G^- and G^+ are homogeneous

solutions, and that G vanishes when t or t' is t_a or t_b . Another form for G is shown in the main text (Equation 13).

Particle in a Potential

Let us concentrate on the case of a particle in a potential in one dimension, with Lagrangian $L = m\dot{q}^2/2 - V(q)$. The dynamical equation is

$$\ddot{q}_c(t) + m^{-1} V'[q_c(t)] = 0. \quad (A13)$$

The small-disturbance equation is:

$$\left[-\frac{d^2}{dt^2} - m^{-1} V''[q_c(t)] \right] f(t) = 0. \quad (A14)$$

Consider two linearly independent solutions of (A14), D and \bar{D} , satisfying:

$$\begin{aligned} D(t_b) &= 1 & \bar{D}(t_b) &= 0 \\ \dot{D}(t_b) &= 0 & \dot{\bar{D}}(t_b) &= -1 \end{aligned} \quad (A15)$$

Their Wronskian $W = \dot{D}\bar{D} - D\dot{\bar{D}}$ is constant and equal to -1 . D and \bar{D} depend on t_b , t_a , q_b and q_a through $q_c(t)$. The antisymmetric Jacobi commutator along the classical path $q_c(t)$ can be shown to be:

$$J(t, t') = \bar{D}(t) D(t') - D(t) \bar{D}(t').$$

It is obviously a solution of (A14) in both t and t' .

Classical path in terms of Jacobi fields

$$q_c(t) = A \int_{t_a}^t D(s) ds + B \int_{t_a}^t \bar{D}(s) ds + q_a$$

where

$$A \equiv \frac{q_b - q_a - V'(q_b) \int_T \bar{D}(u) du}{\int_T D(s) ds} \quad B \equiv V'(q_b). \quad (A16)$$

Proof. $\dot{q}_c(t)$, being a derivative of the classical path, is a solution of the small-disturbance equation, and hence a linear combination of D and \bar{D} : $\dot{q}_c(t) = A D(t) + B \bar{D}(t)$. Integrating from t_a to t yields:

$$q_c(t) = A \int_{t_a}^t D(s) ds + B \int_{t_a}^t \bar{D}(s) ds + q_c(t_a).$$

However, $q_c(t)$ is now the solution of a third-order differential equation. Therefore, we need a third boundary condition, other than $q_c(t_a) = q_a$ and $q_c(t_b) = q_b$. It is provided by the dynamical equation (A13) evaluated, say, at t_b . This gives A and B . Note that:

$$\dot{q}_c(t_a) = A D(t_a) + B \bar{D}(t_a) \quad (A17)$$

$$\dot{q}_c(t_b) = A. \quad (A18)$$

Criterion for non-existence of a classical path

What must the relationship between t_a, t_b, q_a, q_b be in order for a classical path $q_c(t)$ such that $q_c(t_a) = q_a, q_c(t_b) = q_b$ not to exist? The answer is given in terms of Jacobi fields. q_c will not exist if:

$$\left. \begin{array}{l} \text{a) } \int_T D(s) ds = 0, \text{ or } \bar{D}(t_a) = M^{-1} = 0 \\ \text{AND b) } q_b - q_a - V'(q_b) \int_T \bar{D}(s) ds \neq 0 \end{array} \right\} \quad (A19)$$

This is easily proved by looking at (A16) which gives $q_c(t)$ in terms of the Jacobi fields. $q_c(t)$ is infinite if the denominator of A is zero (first condition) and the numerator of A is nonzero (second condition). That the two forms of the first condition are equivalent can be seen by differentiating (A17) with respect to q_b . On the right hand side, we get $\partial \dot{q}_c(t_a) / \partial q_b = M = 1/\bar{D}(t_a)$, and on the left hand side we get a fraction with denominator $(\int_T D(s) ds)^2$. Thus, whenever $\bar{D}(t_a)$ vanishes, $\int_T D(s) ds$ must also vanish.

For a general discussion of these conditions in the context of caustics and catastrophe theory, see Ref. 19.

Zero Jacobi field. The only Jacobi field vanishing at both t_a and t_b is $f(t) = 0$, unless

$$\left. \begin{array}{l} \text{a) } \bar{D}(t_a) = M^{-1} = 0 \\ \text{AND b) } q_b - q_a - V'(q_b) \int_T \bar{D}(s) ds = 0 \end{array} \right\} \quad (A20)$$

in which case $f(t) = a\bar{D}(t)$, where a is an arbitrary constant.

Proof. It is obtained by writing $f(t) = a\bar{D}(t) + bD(t)$ and putting in the boundary conditions. However, if $\bar{D}(t_a) = 0$, we may not have a classical path, in which case a Jacobi field is meaningless. Therefore the second condition is necessary to insure that one or more classical paths might exist.

Example: The harmonic oscillator

We illustrate this with the harmonic oscillator ($V(q) = \frac{1}{2} \omega^2 q^2$).

The classical path, for arbitrary endpoints, is given by:

$$q_c(t) = \frac{q_a \sin \omega(t_b - t) + q_b \sin \omega(t - t_a)}{\sin \omega T} = A \cos(\omega t + \varphi)$$

where $T = t_b - t_a$ and

$$\left\{ \begin{array}{l} A = (\sin \omega T)^{-1} [q_a^2 + q_b^2 - 2q_a q_b \cos \omega T]^{1/2} \\ \varphi = \text{Arc cos} \left(\frac{q_a \sin \omega t_b - q_b \sin \omega t_a}{[q_a^2 + q_b^2 - 2q_a q_b \cos \omega T]^{1/2}} \right) \end{array} \right.$$

It may fail to exist when $\sin(\omega T) = 0$ (the amplitude becomes infinite), except when $q_a = q_b = 0$, in which case there is an infinite number of q_c 's.

The various cases are summarized in Table A1.

The Jacobi fields in this case are:

$$D(t) = \cos \omega(t_b - t) \quad \bar{D}(t) = \frac{1}{\omega} \sin \omega(t_b - t)$$

We can quickly verify all our criteria. We have:

$$(a) \int_T D(s) ds = \bar{D}(t_a) = \frac{1}{\omega} \sin \omega T$$

$$(b) \int_T \bar{D}(s) ds = \frac{1}{\omega^2} (1 - \cos \omega T)$$

If $\omega T = n\pi$, we have no classical path, unless:

$$q_b - q_a - V'(q_b) \omega^{-2} (1 - \cos \omega T) = 0$$

i.e. if $q_a = q_b$ and $\omega T = 2n\pi$ (yielding one path), or if $q_a = q_b = 0$, which implies that $V'(q_b) = 0$ (yielding an infinite number of paths).

Harmonic Oscillator	$q_a \neq q_b$	$q_a = q_b = q_0 \neq 0$	$q_a = q_b = 0$
$\omega T \neq n\pi$	Unique $q_c(t)$ exists and is given by (5.89)	$q_c(t) = q_0 \frac{\cos \omega(t - \frac{t_a+t_b}{2})}{\cos(\frac{\omega T}{2})}$	$q_c(t) = 0$
$\omega T = 2n\pi$	$q_c(t)$ never exists	$q_c(t) = q_0 \frac{\cos \omega(t - \frac{t_a+t_b}{2})}{\cos(n\pi)}$	Noncountably infinite number of classical paths given by:
$\omega T = (2n+1)\pi$	$q_c(t)$ never exists	$q_c(t)$ never exists	$q_c(t) = A \sin \omega(t_b - t)$ (A arbitrary)

Table A1. Classical Paths for the Harmonic Oscillator ($n = \dots, -1, 0, 1, 2, \dots$)

The Commutator Function

The dynamical equation (A13) can be solved by quadratures: If we substitute $\dot{q}_c(t) = u$, we obtain the energy $E \equiv \frac{1}{2} m u^2 + V(q_c) = \text{const.}$ as a first integral. A second integration gives:

$$F(t, t_a, q_c, q_a, E) \equiv t - t_a - \sqrt{\frac{m}{2}} \int_{q_a}^{q_c} \frac{dx}{\sqrt{E - V(x)}} = 0,$$

which yields $t(q_c)$ rather than $q_c(t)$. In order to differentiate the classical path with respect to the constants of integration (here, the energy E and the initial position q_a), we will need the implicit function theorem. The latter states essentially that:

$$F(x_1, \dots, x_n) = 0 \Rightarrow \frac{\partial x_i}{\partial x_j} = - \frac{\partial F / \partial x_j}{\partial F / \partial x_i} \quad (i \neq j).$$

This gives

$$(a) \quad \frac{\partial q_c}{\partial q_a} = \sqrt{\frac{E - V(q_c)}{E - V(q_a)}}$$

$$(b) \quad \frac{\partial q_c}{\partial E} = \frac{1}{2} \sqrt{E - V(q_c)} \int_{q_a}^{q_c} [E - V(x)]^{-3/2} dx$$

(A21)

$$(c) \quad \frac{\partial q_c}{\partial t} = \dot{q}_c(t) = \sqrt{\frac{2}{m} [E - V(q_c)]}$$

$$(d) \quad \frac{\partial q_c}{\partial t_a} = - \sqrt{\frac{2}{m} [E - V(q_c)]}$$

$$(e) \frac{\partial \dot{q}_c(t_b)}{\partial E} = \left(\frac{\partial}{\partial E} \frac{\partial q_c}{\partial t} \right)_{t=t_b} = \left\{ 2m [E - V(q_c(t_b))] \right\}^{-1/2}$$

$$(f) \frac{\partial \dot{q}_c(t_b)}{\partial q_a} = \left(\frac{\partial}{\partial q_a} \frac{\partial q_c}{\partial t} \right)_{t=t_b} = 0$$

Substituting these in (A10), we obtain the commutator (here $p_c = m\dot{q}_c$, $\alpha_1 = q_a$, $\alpha_2 = E$):

$$J(t, t') = \sqrt{\frac{[E - V(q_c(t))][E - V(q_c(t'))]}{2m}} \int_{q_c(t)}^{q_c(t')} \frac{dx}{[E - V(x)]^{3/2}} \quad (A22)$$

If the constants of integration are initial position and momentum q_a and p_a , then $J(t, t')$ is still given by (A22) with E replaced by $p_a^2/2m + V(q_a)$. This is not a trivial statement (compare with (A26)), as we show below.

Proof. In terms of q_a and p_a , the solution is

$$F(t, t_a, q_c, q_a, p_a) \equiv t - t_a - \sqrt{\frac{m}{2}} \int_{q_a}^{q_c} \left[\frac{p_a^2}{2m} + V(q_a) - V(x) \right]^{-1/2} dx = 0 \quad (A23)$$

Then

$$\begin{aligned} \frac{\partial q_c}{\partial q_a} &= - \frac{\partial F / \partial q_a}{\partial F / \partial q_c} \\ &= \left[\frac{p_a^2}{2m} + V(q_a) - V(q_c) \right]^{1/2} \left\{ \frac{\sqrt{2m}}{p_a} + \frac{V'(q_a)}{2} \int_{q_a}^{q_c} \left[\frac{p_a^2}{2m} + V(q_a) - V(x) \right]^{-3/2} dx \right\} \end{aligned}$$

$$\begin{aligned} \frac{\partial q_c}{\partial p_a} &= - \frac{\partial F / \partial p_a}{\partial F / \partial q_c} \\ &= \frac{p_a}{2m} \left\{ \frac{p_a^2}{2m} + V(q_a) - V(q_c) \right\}^{1/2} \int_{q_a}^{q_c} \left\{ \frac{p_a^2}{2m} + V(q_a) - V(x) \right\}^{-3/2} dx \quad (A24) \end{aligned}$$

Substituting the above in expression (15) for J , some terms cancel out and we get the result. The non-triviality of this result is illustrated by the fact that $\partial q_c / \partial q_a$ in (A24) is not obtained from $\partial q_c / \partial q_a$ in (A21a) by simply replacing E by $p_a^2 / 2m + V(q_a)$.

We can give the commutator in terms of the endpoints q_a and q_b . For this we have:

$$\begin{cases} F(t, t_a, q_c, q_a, E) \equiv t - t_a - \sqrt{\frac{m}{2}} \int_{q_a}^{q_c} [E - V(x)]^{-1/2} dx \\ G(t_b, t_a, q_b, q_a, E) \equiv t_b - t_a - \sqrt{\frac{m}{2}} \int_{q_a}^{q_b} [E - V(x)]^{-1/2} dx, \end{cases} \quad (A25)$$

that is, E in the first equation is really a function of q_a and q_b , given implicitly by the second equation. It is no longer an independent constant of integration, but q_b is. Thus, we have:

$$\frac{\partial q_c}{\partial q_a} = - \frac{\frac{\partial F}{\partial q_a}}{\frac{\partial F}{\partial q_c}} = - \frac{\sqrt{\frac{m}{2}} \{E - V(q_a)\}^{-1/2} + \frac{1}{2} \sqrt{\frac{m}{2}} \frac{\partial E}{\partial q_a} \int_{q_a}^{q_c} [E - V(x)]^{-3/2} dx}{-\sqrt{\frac{m}{2}} [E - V(q_c)]^{-1/2}}$$

where $\partial E / \partial q_a$ is obtained by using the implicit function theorem on G :

$$\frac{\partial E}{\partial q_a} = - \frac{\partial G / \partial q_a}{\partial G / \partial E} = \frac{-2}{\sqrt{E - V(q_a)}} \left\{ \int_{q_a}^{q_c} [E - V(x)]^{-3/2} dx \right\}^{-1}$$

Finally,

$$\frac{\partial q_c}{\partial q_a} = \left[\frac{E - V(q_c)}{E - V(q_a)} \right]^{1/2} \cdot \frac{\int_{q_c}^{q_b} [E - V(x)]^{-3/2} dx}{\int_{q_a}^{q_b} [E - V(x)]^{-3/2} dx}$$

Similarly, we find:

$$\frac{\partial q_c}{\partial q_b} = \left[\frac{E - V(q_c)}{E - V(q_b)} \right]^{1/2} \int_{q_a}^{q_c} [E - V(x)]^{-3/2} dx / \int_{q_a}^{q_b} [E - V(x)]^{-3/2} dx$$

As for the Van Vleck - Morette function $M = -m \partial \dot{q}_c(t_b) / \partial q_a$, we use:

$$\dot{q}_c(t_b) = \left[\frac{2}{m} \{E(q_a, q_b) - V(q_b)\} \right]^{1/2}.$$

This gives:

$$M = -m \frac{\partial \dot{q}_c(t_b)}{\partial q_a} = -\frac{m}{2} \sqrt{\frac{2}{m}} [E - V(q_b)]^{-1/2} \frac{\partial E}{\partial q_a},$$

i.e.

$$M = \sqrt{\frac{m}{2}} \left\{ [E - V(q_a)][E - V(q_b)] \right\}^{-1/2} / \int_{q_a}^{q_b} [E - V(x)]^{-3/2} dx.$$

Finally, the commutator in terms of the endpoints is given by (A10) with $x_1 = q_a$ and $x_2 = q_b$:

$$\begin{aligned} J(t, t') = & \left(\frac{2}{m} \right)^{1/2} \sqrt{E - V(q_c(t))} \sqrt{E - V(q_c(t'))} \left[\int_{q_a}^{q_b} \{E - V(x)\}^{-3/2} dx \right]^{-1} \\ & \times \left\{ \int_{q_c(t)}^{q_b} dx [E - V(x)]^{-3/2} \int_{q_a}^{q_c(t')} dy [E - V(y)]^{-3/2} - \right. \\ & \left. - \int_{q_c(t')}^{q_b} dx [E - V(x)]^{-3/2} \int_{q_a}^{q_c(t)} dy [E - V(y)]^{-3/2} \right\}, \quad (A26) \end{aligned}$$

where $q_c(t, q_a, q_b)$ and $E(q_a, q_b)$ are given implicitly by (A25).

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